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# *N*′-[(*E*)-4-Benzyloxy-2-hydroxybenzylidene]benzohydrazide

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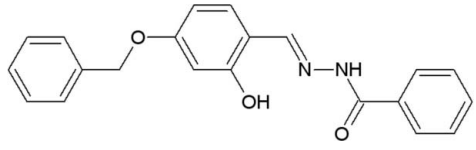
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.029; $wR$ factor = 0.082; data-to-parameter ratio = 7.0.

The title compound, $C_{21}H_{18}N_2O_3$, exists in the *E* conformation with respect to the azomethane C=N double bond. The central benzene ring is almost coplanar with one of the substituent benzene rings [dihedral angle = 1.74 (5)°] and is approximately orthogonal to the other benzene ring of the molecule [dihedral angle = 86.61 (7)°]. An intramolecular O—H···N hydrogen bond occurs. The crystal packing is dominated by N—H···O hydrogen bonds, which lead to an infinite chain running parallel to [010].

## Related literature

For the biological activity of hydrazones, see: Patil *et al.* (2010); Zhang *et al.* (2010). For the synthesis of related compounds, see: Emmanuel *et al.* (2011); Mangalam & Kurup (2011). For related structures, see: Lin & Sang (2009); Mohd Lair *et al.* (2009).




## Experimental

### *Crystal data*

$C_{21}H_{18}N_2O_3$
$M_r$ = 346.37
Monoclinic, $P2_1$
$a$ = 10.8053 (6) Å
$b$ = 4.8952 (2) Å
$c$ = 16.3601 (10) Å
$\beta$ = 95.813 (2)°
$V$ = 860.90 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
0.35 × 0.30 × 0.25 mm

### *Data collection*

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.969, $T_{max}$ = 0.978
9033 measured reflections
1705 independent reflections
1593 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.082
$S$ = 1.12
1705 reflections
243 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.12 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2′···O3$^{i}$ | 0.85 (1) | 2.09 (1) | 2.903 (2) | 160 (2) |
| O2—H2″···N1 | 0.87 (2) | 1.79 (2) | 2.592 (2) | 152 (3) |

Symmetry code: (i) $x, y+1, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2591).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o2785 [doi:10.1107/S1600536812036306]

## *N*′-[(*E*)-4-Benzyloxy-2-hydroxybenzylidene]benzohydrazide

**P. R. Reshma, M. Sithambaresan and M. R. Prathapachandra Kurup**

### Comment

Hydrazone compounds have received much attention due to their potential applications in biological chemistry (Patil *et al.*, 2010; Zhang *et al.*, 2010). As a continuous work on the hydrazone compounds, a new hydrazone compound, *N*′-{(*E*)-[4-(benzyloxy)-2-hydroxyphenyl]methylidene}benzohydrazide, was prepared and structurally characterized. The *ORTEP* view of the title compound is shown in Fig. 1.

The compound crystallizes in monoclinic space group $P2_1$. The molecule adopts an *E* configuration with respect to C14=N1 bond (Lin & Sang 2009; Mohd Lair *et al.*, 2009) and it exists in amido form with C15=O3 bond length of 1.224 (3) Å which is very close to a formal C=O bond length [1.21 Å]. The aromatic ring C8—C13 is almost coplanar with the ring C16—C21 with dihedral angle of 1.74 (5)° whilst the ring C1—C6 is approximately orthogonal (86.61 (7)°) to the ring C16—C21.

While the intramolecular hydrogen bond O(2)—H(2′′)···N(1) increases the rigidity of the molecule, intermolecular N(2)—H(2′)···O(3) hydrogen bond (Table 1) links the adjacent molecules forming an infinite one-dimensional supramolecular chain running parallel to the [010] direction in the unit cell (Fig. 2). Benzohydrazone molecules within these chains also interact through very weak $\pi\cdots\pi$ interactions with a shortest centroid-centroid distance of 4.8950 (15) Å that not only augment the stronger N—H···O hydrogen bond but also interconnects the infinite chains forming three-dimensional network in the lattice. The parallel arrangement of the molecules along *b* axis is shown in Fig. 3.

### Experimental

The title compound was prepared by adapting a reported procedure (Emmanuel *et al.*, 2011; Mangalam & Kurup, 2011) by refluxing a mixture of methanolic solutions of benzhydrazide (0.136 g,1 mmol) and 4-benzyloxysalicylaldehyde (0.2282 g,1 mmol) for 4 h. The formed crystals were collected, washed with few drops of methanol and dried over $P_4O_{10}$ *in vacuo*. Single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation from its methanolic solution.

### Refinement

All H atoms on C were placed in calculated positions, guided by difference maps, with C—H bond distances 0.93–0.97 Å. H atoms were assigned as $U_{iso}$=1.2Ueq. H atoms of O2—H2′′ and N2—H2′ bonds were located from difference maps and restrained using *DFIX* instructions with O—H = 0.87 ± 0.02 Å and N—H = 0.85 ± 0.01 Å.

In the absence of significant anomalous scattering effects Friedel pairs have been merged.

### Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012) and *DIAMOND* (Brandenburg,

2010); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

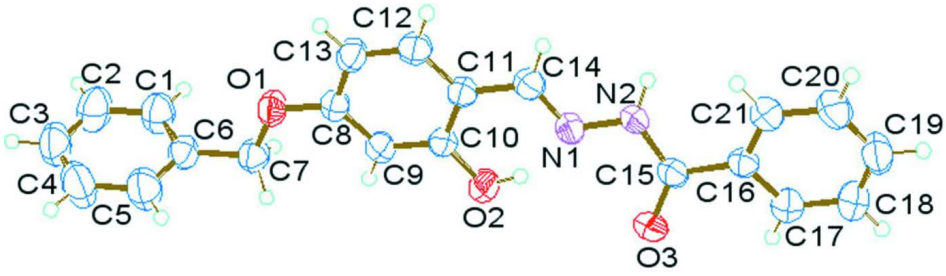


**Figure 1**

*ORTEP* view of the unique part of the compound, drawn with 50% probability displacement ellipsoids for the non-H atoms.

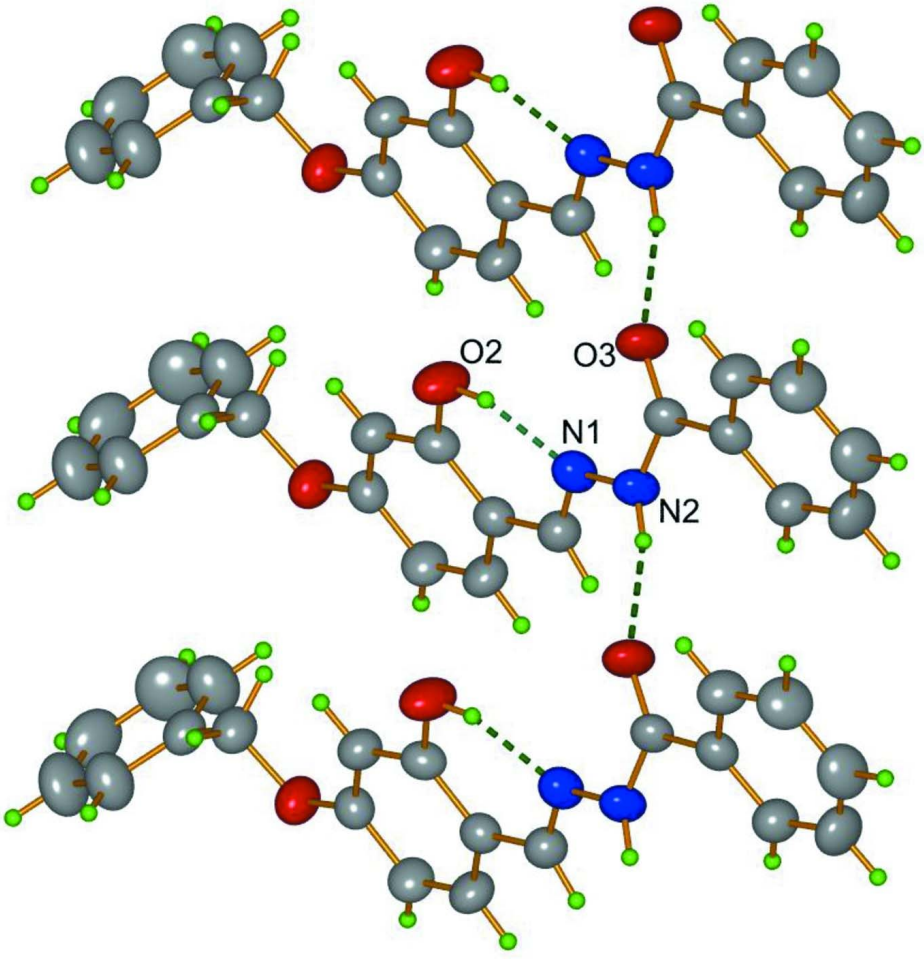


**Figure 2**

Graphical representation showing one-dimensional supramolecular hydrogen bonding network in the crystal structure of $C_{21}H_{18}N_2O_3$.

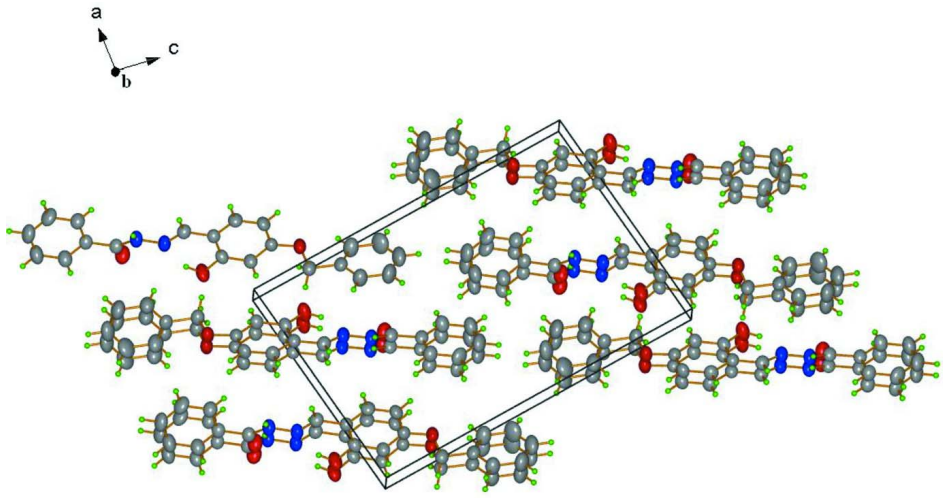


**Figure 3**

Packing diagram of the compound showing the parallel arrangement of the molecules along *b* axis.

### *N*′-[(*E*)-4-Benzyloxy-2-hydroxybenzylidene]benzohydrazide

*Crystal data*

$C_{21}H_{18}N_2O_3$
$M_r$ = 346.37
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a$ = 10.8053 (6) Å
$b$ = 4.8952 (2) Å
$c$ = 16.3601 (10) Å
$\beta$ = 95.813 (2)°
$V$ = 860.90 (8) Å$^3$
$Z$ = 2
$F(000)$ = 364
$D_x$ = 1.336 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5951 reflections
$\theta$ = 2.4–28.1°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
Block, colorless
0.35 × 0.30 × 0.25 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm$^{-1}$
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.969, $T_{max}$ = 0.978
9033 measured reflections
1705 independent reflections
1593 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 3.0°
$h$ = −12→12
$k$ = −5→5
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.082
$S$ = 1.12
1705 reflections
243 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.0573P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$

$\Delta\rho_{max} = 0.12$ e Å$^{-3}$
$\Delta\rho_{min} = -0.14$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.08187 (12) | 0.6299 (3) | 1.18699 (7) | 0.0525 (4) |
| O2 | 0.19313 (15) | 0.4504 (4) | 0.91841 (8) | 0.0610 (4) |
| O3 | 0.43474 (14) | 0.3828 (3) | 0.76116 (9) | 0.0575 (4) |
| N1 | 0.37436 (15) | 0.7368 (4) | 0.87075 (9) | 0.0471 (4) |
| N2 | 0.44743 (17) | 0.8127 (3) | 0.81016 (10) | 0.0458 (4) |
| C1 | −0.1620 (2) | 0.5457 (6) | 1.27899 (13) | 0.0681 (7) |
| H1 | −0.1984 | 0.6716 | 1.2413 | 0.082* |
| C2 | −0.2072 (2) | 0.5169 (8) | 1.35467 (15) | 0.0812 (9) |
| H2A | −0.2737 | 0.6235 | 1.3677 | 0.097* |
| C3 | −0.1550 (3) | 0.3347 (7) | 1.40967 (15) | 0.0779 (8) |
| H3 | −0.1853 | 0.3174 | 1.4607 | 0.093* |
| C4 | −0.0583 (3) | 0.1761 (8) | 1.39081 (16) | 0.0890 (9) |
| H4 | −0.0228 | 0.0501 | 1.4288 | 0.107* |
| C5 | −0.0126 (2) | 0.2025 (7) | 1.31467 (15) | 0.0750 (7) |
| H5 | 0.0528 | 0.0928 | 1.3015 | 0.090* |
| C6 | −0.06386 (17) | 0.3899 (5) | 1.25910 (11) | 0.0500 (5) |
| C7 | −0.01383 (18) | 0.4243 (5) | 1.17735 (11) | 0.0531 (5) |
| H7A | 0.0203 | 0.2531 | 1.1600 | 0.064* |
| H7B | −0.0798 | 0.4808 | 1.1361 | 0.064* |
| C8 | 0.14629 (15) | 0.6828 (4) | 1.12181 (10) | 0.0424 (4) |
| C9 | 0.13243 (17) | 0.5416 (4) | 1.04847 (11) | 0.0464 (5) |
| H9 | 0.0725 | 0.4054 | 1.0401 | 0.056* |
| C10 | 0.20779 (17) | 0.6026 (4) | 0.98724 (10) | 0.0431 (4) |
| C11 | 0.29517 (17) | 0.8163 (4) | 0.99739 (10) | 0.0421 (4) |
| C12 | 0.30438 (17) | 0.9593 (5) | 1.07174 (11) | 0.0501 (5) |
| H12 | 0.3604 | 1.1034 | 1.0794 | 0.060* |
| C13 | 0.23345 (17) | 0.8937 (5) | 1.13355 (11) | 0.0493 (5) |
| H13 | 0.2431 | 0.9886 | 1.1830 | 0.059* |
| C14 | 0.37200 (17) | 0.8897 (5) | 0.93334 (11) | 0.0470 (4) |
| H14 | 0.4195 | 1.0484 | 0.9380 | 0.056* |
| C15 | 0.47098 (17) | 0.6182 (4) | 0.75527 (11) | 0.0427 (4) |
| C16 | 0.54733 (16) | 0.7030 (4) | 0.68911 (11) | 0.0433 (4) |
| C17 | 0.5333 (2) | 0.5618 (5) | 0.61561 (12) | 0.0565 (6) |

| | | | | |
|---|---|---|---|---|
| H17 | 0.4738 | 0.4244 | 0.6077 | 0.068* |
| C18 | 0.6065 (2) | 0.6223 (6) | 0.55402 (13) | 0.0671 (6) |
| H18 | 0.5957 | 0.5273 | 0.5046 | 0.080* |
| C19 | 0.6950 (2) | 0.8216 (6) | 0.56521 (14) | 0.0673 (7) |
| H19 | 0.7449 | 0.8610 | 0.5236 | 0.081* |
| C20 | 0.7105 (2) | 0.9643 (6) | 0.63802 (14) | 0.0655 (6) |
| H20 | 0.7709 | 1.0998 | 0.6455 | 0.079* |
| C21 | 0.63653 (18) | 0.9069 (5) | 0.70001 (13) | 0.0532 (5) |
| H21 | 0.6466 | 1.0048 | 0.7489 | 0.064* |
| H2′ | 0.4593 (19) | 0.9831 (9) | 0.8048 (13) | 0.047 (6)* |
| H2″ | 0.249 (2) | 0.514 (7) | 0.8883 (16) | 0.100 (10)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0541 (7) | 0.0627 (10) | 0.0425 (6) | −0.0105 (7) | 0.0144 (5) | −0.0043 (7) |
| O2 | 0.0859 (10) | 0.0528 (10) | 0.0474 (7) | −0.0177 (8) | 0.0207 (7) | −0.0110 (7) |
| O3 | 0.0747 (9) | 0.0345 (8) | 0.0668 (9) | −0.0058 (7) | 0.0238 (7) | 0.0026 (7) |
| N1 | 0.0560 (9) | 0.0423 (10) | 0.0454 (8) | 0.0030 (8) | 0.0161 (7) | 0.0061 (8) |
| N2 | 0.0602 (9) | 0.0320 (9) | 0.0478 (8) | 0.0002 (7) | 0.0184 (7) | 0.0059 (7) |
| C1 | 0.0652 (12) | 0.0807 (18) | 0.0605 (12) | 0.0120 (13) | 0.0162 (10) | 0.0076 (13) |
| C2 | 0.0728 (15) | 0.103 (2) | 0.0724 (15) | 0.0086 (16) | 0.0311 (12) | −0.0023 (17) |
| C3 | 0.0884 (17) | 0.090 (2) | 0.0604 (13) | −0.0181 (17) | 0.0300 (12) | 0.0016 (15) |
| C4 | 0.106 (2) | 0.094 (2) | 0.0688 (15) | 0.0056 (19) | 0.0186 (14) | 0.0313 (17) |
| C5 | 0.0768 (15) | 0.0803 (19) | 0.0712 (14) | 0.0118 (14) | 0.0235 (12) | 0.0150 (14) |
| C6 | 0.0466 (10) | 0.0556 (12) | 0.0488 (9) | −0.0096 (10) | 0.0094 (8) | −0.0032 (10) |
| C7 | 0.0530 (10) | 0.0581 (14) | 0.0497 (10) | −0.0071 (11) | 0.0115 (8) | −0.0053 (10) |
| C8 | 0.0418 (9) | 0.0464 (12) | 0.0396 (9) | 0.0028 (8) | 0.0060 (7) | 0.0006 (9) |
| C9 | 0.0505 (10) | 0.0439 (11) | 0.0454 (10) | −0.0058 (9) | 0.0078 (8) | 0.0003 (9) |
| C10 | 0.0536 (10) | 0.0382 (10) | 0.0377 (8) | 0.0020 (9) | 0.0059 (7) | 0.0002 (8) |
| C11 | 0.0447 (9) | 0.0407 (11) | 0.0414 (9) | 0.0028 (8) | 0.0061 (7) | 0.0016 (8) |
| C12 | 0.0504 (10) | 0.0492 (13) | 0.0508 (10) | −0.0105 (10) | 0.0055 (8) | −0.0052 (9) |
| C13 | 0.0542 (10) | 0.0547 (12) | 0.0391 (9) | −0.0051 (10) | 0.0055 (7) | −0.0061 (10) |
| C14 | 0.0487 (9) | 0.0425 (11) | 0.0507 (10) | −0.0011 (9) | 0.0091 (8) | 0.0022 (10) |
| C15 | 0.0482 (10) | 0.0349 (10) | 0.0460 (9) | 0.0024 (9) | 0.0089 (7) | 0.0057 (9) |
| C16 | 0.0482 (10) | 0.0364 (10) | 0.0465 (9) | 0.0053 (8) | 0.0097 (8) | 0.0052 (8) |
| C17 | 0.0673 (12) | 0.0523 (14) | 0.0515 (11) | −0.0063 (11) | 0.0139 (9) | −0.0026 (10) |
| C18 | 0.0844 (15) | 0.0710 (17) | 0.0487 (11) | −0.0028 (15) | 0.0210 (10) | −0.0012 (12) |
| C19 | 0.0731 (14) | 0.0721 (17) | 0.0613 (13) | 0.0023 (13) | 0.0296 (11) | 0.0135 (13) |
| C20 | 0.0601 (12) | 0.0620 (16) | 0.0779 (15) | −0.0129 (12) | 0.0245 (10) | 0.0058 (13) |
| C21 | 0.0565 (10) | 0.0488 (12) | 0.0558 (10) | −0.0040 (10) | 0.0131 (8) | 0.0003 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C8 | 1.356 (2) | C8—C9 | 1.380 (3) |
| O1—C7 | 1.440 (3) | C8—C13 | 1.397 (3) |
| O2—C10 | 1.346 (2) | C9—C10 | 1.386 (3) |
| O2—H2″ | 0.871 (18) | C9—H9 | 0.9300 |
| O3—C15 | 1.224 (3) | C10—C11 | 1.407 (3) |
| N1—C14 | 1.271 (2) | C11—C12 | 1.398 (3) |

| | | | |
|---|---|---|---|
| N1—N2 | 1.379 (2) | C11—C14 | 1.447 (2) |
| N2—C15 | 1.350 (3) | C12—C13 | 1.367 (3) |
| N2—H2′ | 0.8500 (11) | C12—H12 | 0.9300 |
| C1—C6 | 1.372 (3) | C13—H13 | 0.9300 |
| C1—C2 | 1.383 (3) | C14—H14 | 0.9300 |
| C1—H1 | 0.9300 | C15—C16 | 1.485 (2) |
| C2—C3 | 1.349 (4) | C16—C17 | 1.382 (3) |
| C2—H2A | 0.9300 | C16—C21 | 1.386 (3) |
| C3—C4 | 1.363 (4) | C17—C18 | 1.375 (3) |
| C3—H3 | 0.9300 | C17—H17 | 0.9300 |
| C4—C5 | 1.392 (3) | C18—C19 | 1.365 (4) |
| C4—H4 | 0.9300 | C18—H18 | 0.9300 |
| C5—C6 | 1.369 (4) | C19—C20 | 1.376 (3) |
| C5—H5 | 0.9300 | C19—H19 | 0.9300 |
| C6—C7 | 1.502 (2) | C20—C21 | 1.382 (3) |
| C7—H7A | 0.9700 | C20—H20 | 0.9300 |
| C7—H7B | 0.9700 | C21—H21 | 0.9300 |

| | | | |
|---|---|---|---|
| C8—O1—C7 | 117.87 (14) | O2—C10—C9 | 117.22 (18) |
| C10—O2—H2″ | 104 (2) | O2—C10—C11 | 122.05 (16) |
| C14—N1—N2 | 118.70 (17) | C9—C10—C11 | 120.73 (17) |
| C15—N2—N1 | 116.64 (16) | C12—C11—C10 | 117.55 (16) |
| C15—N2—H2′ | 125.7 (15) | C12—C11—C14 | 120.68 (18) |
| N1—N2—H2′ | 116.2 (15) | C10—C11—C14 | 121.77 (17) |
| C6—C1—C2 | 120.5 (2) | C13—C12—C11 | 121.99 (19) |
| C6—C1—H1 | 119.8 | C13—C12—H12 | 119.0 |
| C2—C1—H1 | 119.8 | C11—C12—H12 | 119.0 |
| C3—C2—C1 | 120.2 (3) | C12—C13—C8 | 119.49 (17) |
| C3—C2—H2A | 119.9 | C12—C13—H13 | 120.3 |
| C1—C2—H2A | 119.9 | C8—C13—H13 | 120.3 |
| C2—C3—C4 | 120.3 (2) | N1—C14—C11 | 119.8 (2) |
| C2—C3—H3 | 119.9 | N1—C14—H14 | 120.1 |
| C4—C3—H3 | 119.9 | C11—C14—H14 | 120.1 |
| C3—C4—C5 | 120.0 (3) | O3—C15—N2 | 121.87 (17) |
| C3—C4—H4 | 120.0 | O3—C15—C16 | 121.75 (18) |
| C5—C4—H4 | 120.0 | N2—C15—C16 | 116.34 (18) |
| C6—C5—C4 | 120.0 (3) | C17—C16—C21 | 119.04 (17) |
| C6—C5—H5 | 120.0 | C17—C16—C15 | 118.32 (18) |
| C4—C5—H5 | 120.0 | C21—C16—C15 | 122.54 (18) |
| C5—C6—C1 | 119.1 (2) | C18—C17—C16 | 120.6 (2) |
| C5—C6—C7 | 120.6 (2) | C18—C17—H17 | 119.7 |
| C1—C6—C7 | 120.4 (2) | C16—C17—H17 | 119.7 |
| O1—C7—C6 | 107.46 (16) | C19—C18—C17 | 120.2 (2) |
| O1—C7—H7A | 110.2 | C19—C18—H18 | 119.9 |
| C6—C7—H7A | 110.2 | C17—C18—H18 | 119.9 |
| O1—C7—H7B | 110.2 | C18—C19—C20 | 120.06 (19) |
| C6—C7—H7B | 110.2 | C18—C19—H19 | 120.0 |
| H7A—C7—H7B | 108.5 | C20—C19—H19 | 120.0 |
| O1—C8—C9 | 124.68 (17) | C19—C20—C21 | 120.2 (2) |

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|---|---|---|---|
| O1—C8—C13 | 115.18 (16) | C19—C20—H20 | 119.9 |
| C9—C8—C13 | 120.13 (16) | C21—C20—H20 | 119.9 |
| C8—C9—C10 | 120.04 (18) | C20—C21—C16 | 119.9 (2) |
| C8—C9—H9 | 120.0 | C20—C21—H21 | 120.1 |
| C10—C9—H9 | 120.0 | C16—C21—H21 | 120.1 |
| | | | |
| C14—N1—N2—C15 | 164.71 (18) | C10—C11—C12—C13 | 1.2 (3) |
| C6—C1—C2—C3 | −0.1 (4) | C14—C11—C12—C13 | −179.66 (19) |
| C1—C2—C3—C4 | −0.6 (5) | C11—C12—C13—C8 | −1.9 (3) |
| C2—C3—C4—C5 | 0.3 (5) | O1—C8—C13—C12 | 178.99 (18) |
| C3—C4—C5—C6 | 0.7 (5) | C9—C8—C13—C12 | 0.2 (3) |
| C4—C5—C6—C1 | −1.4 (4) | N2—N1—C14—C11 | 179.39 (16) |
| C4—C5—C6—C7 | 178.8 (3) | C12—C11—C14—N1 | 170.89 (18) |
| C2—C1—C6—C5 | 1.0 (4) | C10—C11—C14—N1 | −10.0 (3) |
| C2—C1—C6—C7 | −179.1 (3) | N1—N2—C15—O3 | −3.6 (3) |
| C8—O1—C7—C6 | 175.83 (17) | N1—N2—C15—C16 | 178.67 (15) |
| C5—C6—C7—O1 | −90.4 (3) | O3—C15—C16—C17 | 28.2 (3) |
| C1—C6—C7—O1 | 89.8 (2) | N2—C15—C16—C17 | −154.05 (19) |
| C7—O1—C8—C9 | −4.4 (3) | O3—C15—C16—C21 | −148.1 (2) |
| C7—O1—C8—C13 | 176.89 (17) | N2—C15—C16—C21 | 29.7 (3) |
| O1—C8—C9—C10 | −176.51 (17) | C21—C16—C17—C18 | −0.1 (3) |
| C13—C8—C9—C10 | 2.1 (3) | C15—C16—C17—C18 | −176.5 (2) |
| C8—C9—C10—O2 | 177.42 (18) | C16—C17—C18—C19 | 0.7 (4) |
| C8—C9—C10—C11 | −2.9 (3) | C17—C18—C19—C20 | −0.6 (4) |
| O2—C10—C11—C12 | −179.1 (2) | C18—C19—C20—C21 | −0.1 (4) |
| C9—C10—C11—C12 | 1.2 (3) | C19—C20—C21—C16 | 0.6 (4) |
| O2—C10—C11—C14 | 1.8 (3) | C17—C16—C21—C20 | −0.5 (3) |
| C9—C10—C11—C14 | −177.93 (18) | C15—C16—C21—C20 | 175.6 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2′···O3$^{i}$ | 0.85 (1) | 2.09 (1) | 2.903 (2) | 160 (2) |
| O2—H2″···N1 | 0.87 (2) | 1.79 (2) | 2.592 (2) | 152 (3) |

Symmetry code: (i) *x*, *y*+1, *z*.